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TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 13	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 41	Jan 21	PHARMAML offering one free connect hour in February 2003
NEWS 42	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 43	Feb 13	CANCERLIT is no longer being updated
NEWS 44	Feb 24	METADEX enhancements
NEWS 45	Feb 24	PCTGEN now available on STN
NEWS 46	Feb 24	TEMA now available on STN
NEWS 47	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 48	Feb 26	PCTFULL now contains images

10/027,644

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 NEWS 49  Mar 04  SDI PACKAGE for monthly delivery of multifile SDI results

 NEWS EXPRESS  January 6 CURRENT WINDOWS VERSION IS V6.01a,
               CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *



FILE 'HOME' ENTERED AT 10:55:00 ON 13 MAR 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:55:17 ON 13 MAR 2003
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STRUCTURE FILE UPDATES:   12 MAR 2003  HIGHEST RN 498527-50-7
DICTIONARY FILE UPDATES:  12 MAR 2003  HIGHEST RN 498527-50-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10027644.str

L1      STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 10:56:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    447 TO ITERATE
```

100.0% PROCESSED 447 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 7672 TO 10208
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 10:56:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9334 TO ITERATE

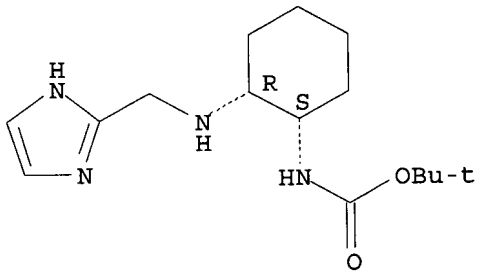
100.0% PROCESSED 9334 ITERATIONS 44 ANSWERS
SEARCH TIME: 00.00.01

L3 44 SEA SSS FUL L1

=> d scan

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Carbamic acid, [(1R,2S)-2-[(1H-imidazol-2-ylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI)
MF C15 H26 N4 O2

Relative stereochemistry.

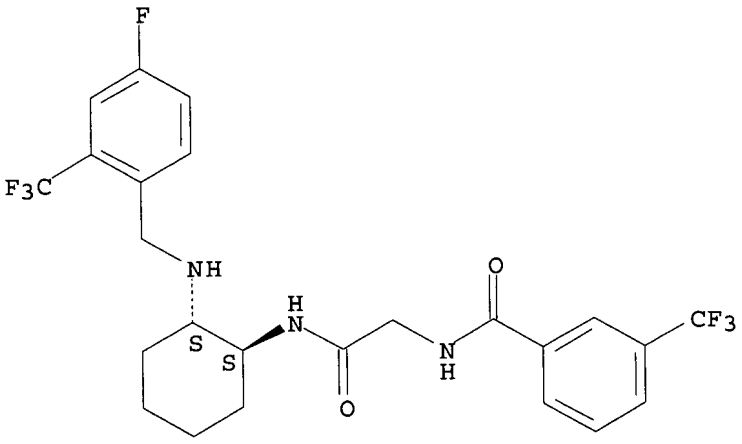


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, N-[2-[[(1S,2S)-2-[[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI)
MF C24 H24 F7 N3 O2

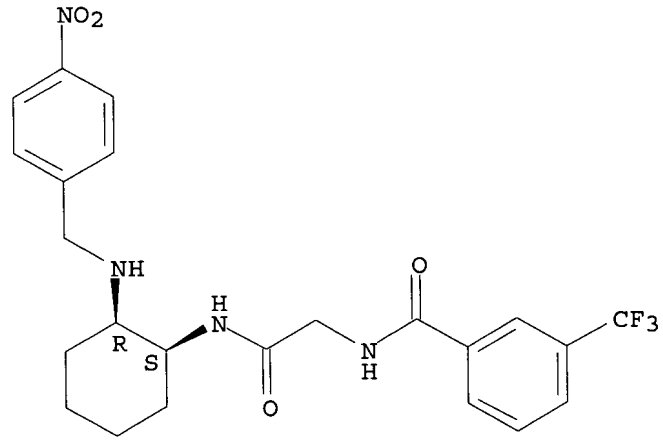
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, N-[2-[[(1R,2S)-2-[[(4-nitrophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI)
MF C23 H25 F3 N4 O4

Relative stereochemistry.

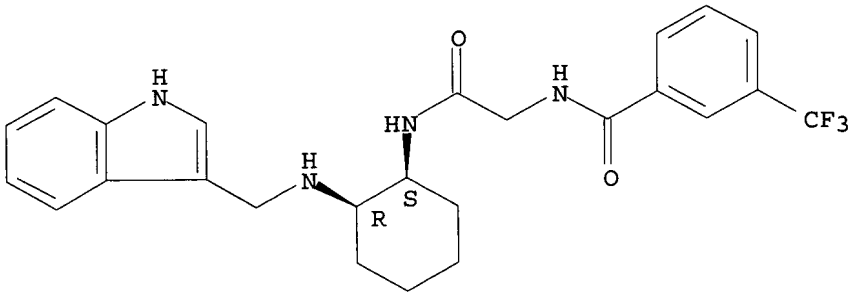


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, N-[2-[[(1R,2S)-2-[(1H-indol-3-ylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI)
MF C25 H27 F3 N4 O2

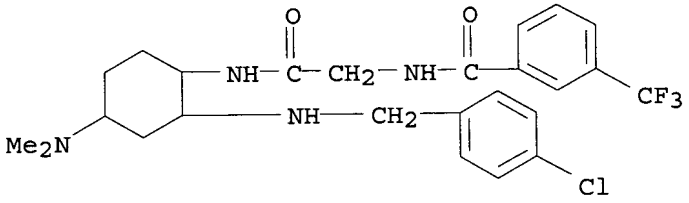
Relative stereochemistry.



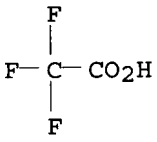
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 44 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, N-[2-[[2-[[(4-chlorophenyl)methyl]amino]-4-(dimethylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI)
MF C25 H30 Cl F3 N4 O2 . x C2 H F3 O2

CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.95	149.16

FILE 'CAPLUS' ENTERED AT 10:56:48 ON 13 MAR 2003
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FILE COVERS 1907 - 13 Mar 2003 VOL 138 ISS 11
FILE LAST UPDATED: 12 Mar 2003 (20030312/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> hist dis
HIST IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> dis his

(FILE 'HOME' ENTERED AT 10:55:00 ON 13 MAR 2003)

FILE 'REGISTRY' ENTERED AT 10:55:17 ON 13 MAR 2003
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 44 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:56:48 ON 13 MAR 2003

=> s l3
L4 8 L3

=> d l4 ibib hitstr abs 1-8

L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:594806 CAPLUS
DOCUMENT NUMBER: 137:154762
TITLE: Preparation of N-[2-(cycloalkylamino)-2-oxoethyl]benzamides and related compounds as modulators of chemokine receptor activity
INVENTOR(S): Cherney, Robert
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

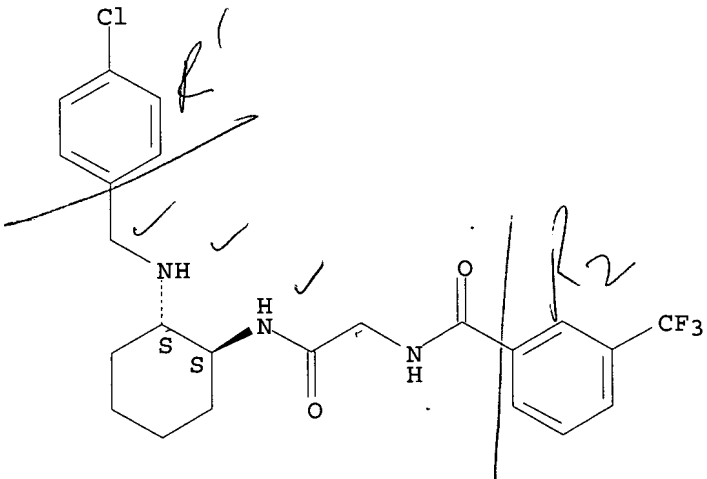
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002060859	A2	20020808	WO 2001-US50252	20011220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004151	A1	20030102	US 2001-27644	20011220
PRIORITY APPLN. INFO.:			US 2000-256904P	P 20001220
OTHER SOURCE(S):		MARPAT 137:154762		

IT **445478-71-7P**, N-[2-[[(1S,2S)-2-[[(4-Chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(chemokine receptor modulator; prepn. of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445478-71-7 CAPLUS

CN Benzamide, N-[2-[[(1S,2S)-2-[[(4-chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

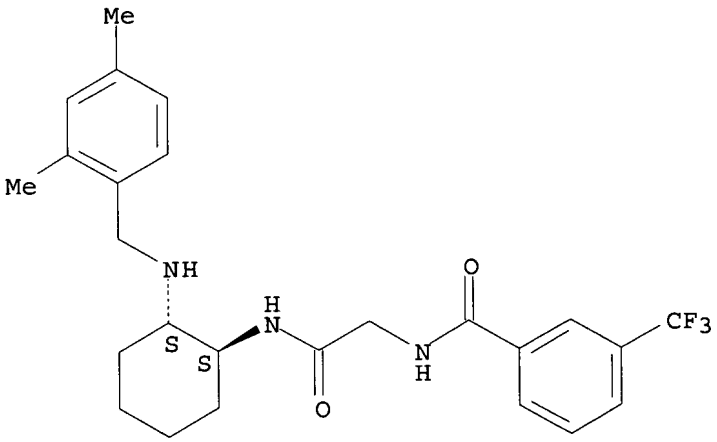


IT **445478-74-0P**, N-[2-[[(1S,2S)-2-[[(2,4-Dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-75-1P**, N-[2-[[(1S,2S)-2-[[(2,4,6-Trimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-76-2P**, N-[2-[[(1S,2S)-2-[[(4-Benzyloxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-77-3P**, N-[2-[[(1S,2S)-2-[[(2,4-Difluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-78-4P**, N-[2-[[(1S,2S)-2-[[(2-Chloro-4-fluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-79-5P**, N-[2-[[(1S,2S)-2-[[(2-Trifluoromethyl-4-fluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-80-8P**, N-[2-[[(1S,2S)-2-[[(2,4-Dichlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-81-9P**, N-[2-[[(1S,2S)-2-[[(2-Fluoro-6-trifluoromethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-82-0P**, N-[2-[[(1S,2S)-2-[[(2-Chloro-5-trifluoromethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-83-1P**, N-[2-[[(1S,2S)-2-[[(1-Naphthyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-87-5P**, N-[2-[[cis-2-[[(2,4-Dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-88-6P**, N-[2-[[cis-2-[[(4-Chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-89-7P**, N-[2-[[cis-2-[[(4-Nitrophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-90-0P**, N-[2-[[cis-2-[[(4-Isopropylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-91-1P**, N-[2-[[cis-2-[[(4-Trifluoromethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-92-2P**, N-[2-[[cis-2-[[(4-Trifluoromethoxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-

(trifluoromethyl)benzamide **445478-93-3P**, N-[2-[[cis-2-[[(4-Phenoxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-94-4P**, N-[2-[[cis-2-[[(1-Naphthyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-95-5P**, N-[2-[[cis-2-[[(2-Naphthyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445478-96-6P**, N-[2-[[cis-2-[[(3-Indolyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445480-70-6P**, 2-Isopropylamino-N-[[[cis-2-(4-methylthiobenzylamino)cyclohexyl]carbamoyl]methyl]-5-(trifluoromethyl)benzamide **445480-72-8P 445480-74-0P 445481-10-7P 445481-16-3P 445481-18-5P 445481-20-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(chemokine receptor modulator; prepn. of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

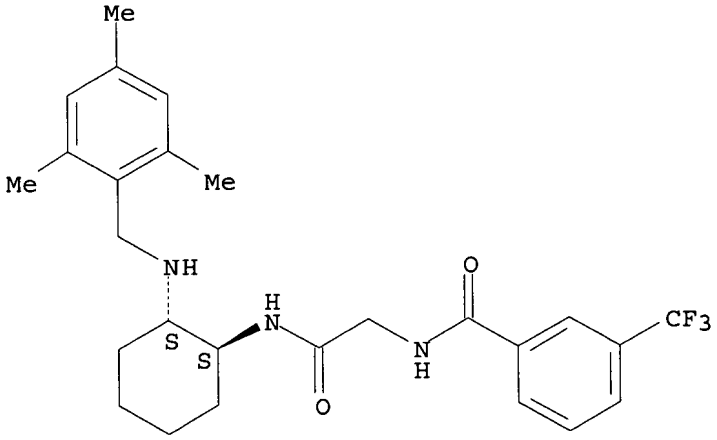
RN 445478-74-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[(2,4-dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



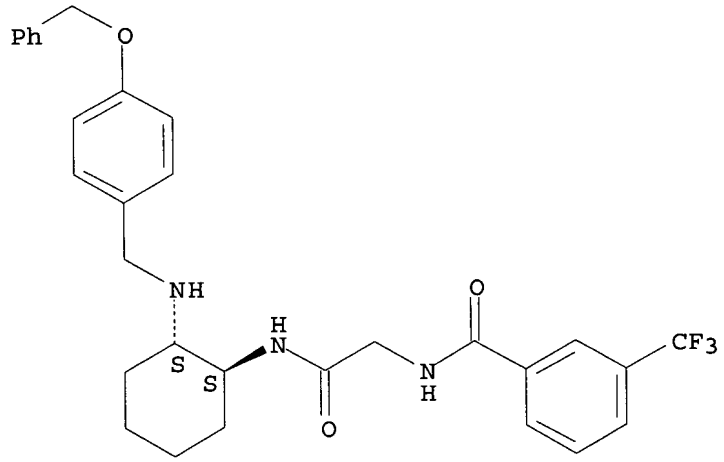
RN 445478-75-1 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1S,2S)-2-[[(2,4,6-trimethylphenyl)methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



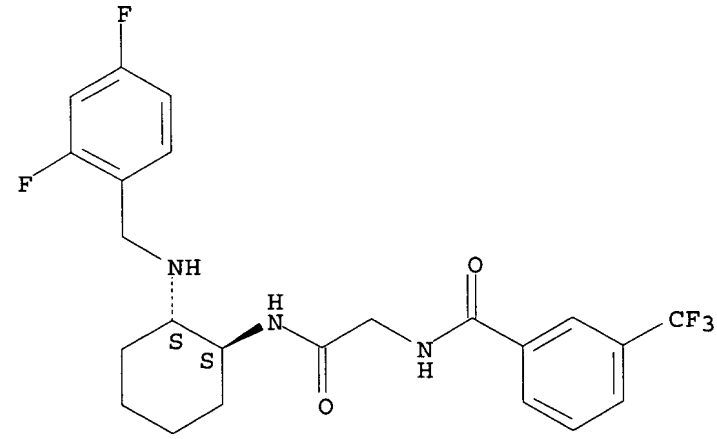
RN 445478-76-2 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1S,2S)-2-[[[4-(phenylmethoxy)phenyl]methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

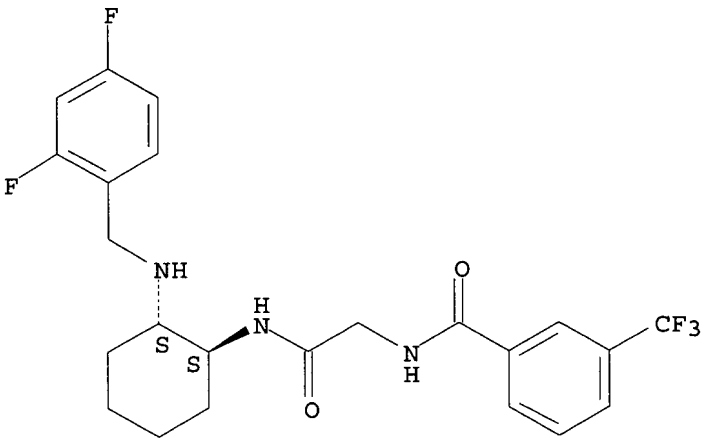
Absolute stereochemistry.



RN 445478-77-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[(2,4-difluorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

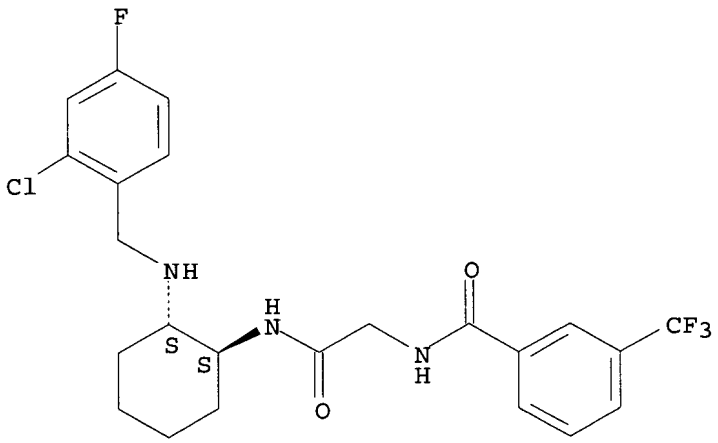
Absolute stereochemistry.





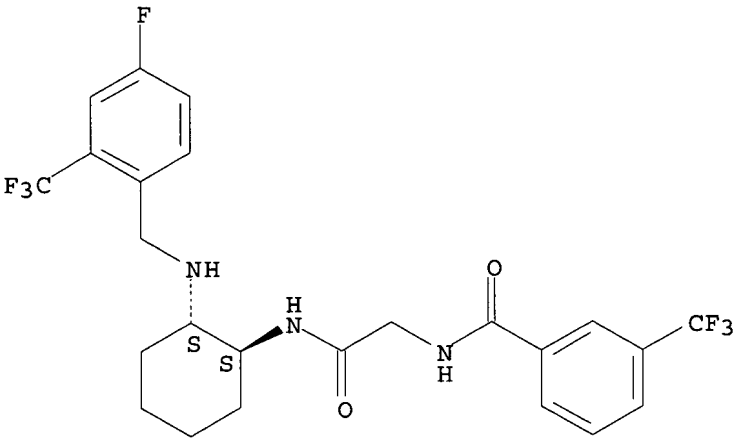
RN 445478-78-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[(2-chloro-4-fluorophenyl)methyl]amino]cycloh
exyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



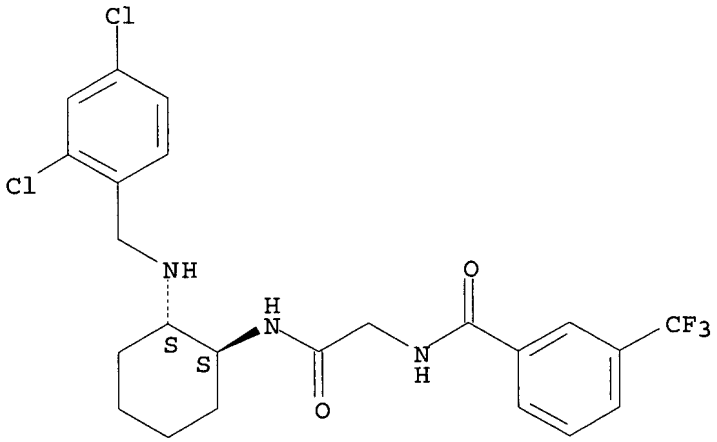
RN 445478-79-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]a
mino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



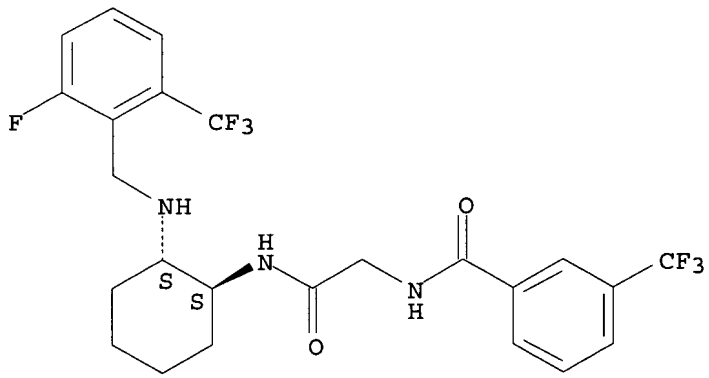
RN 445478-80-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[(2,4-dichlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



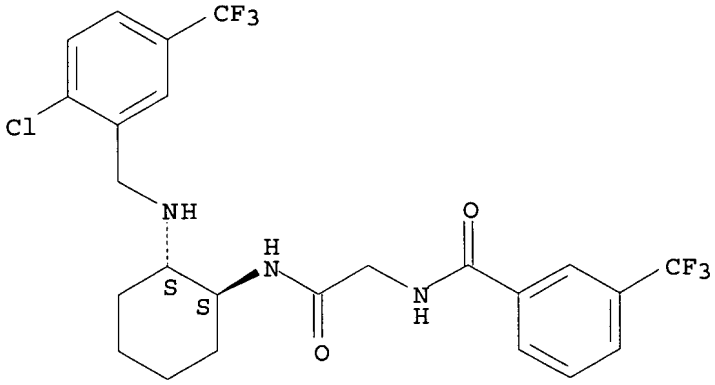
RN 445478-81-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[[2-fluoro-6-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



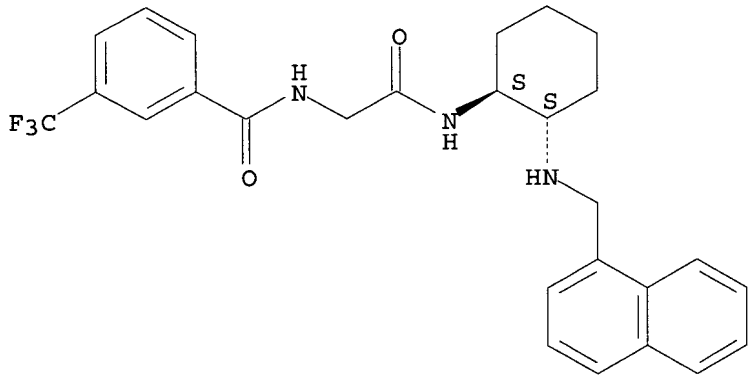
RN 445478-82-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[[[2-chloro-5-(trifluoromethyl)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



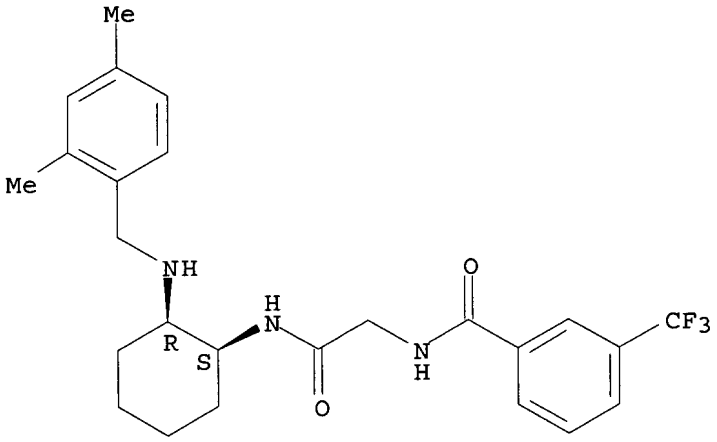
RN 445478-83-1 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-2-[(1-naphthalenylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



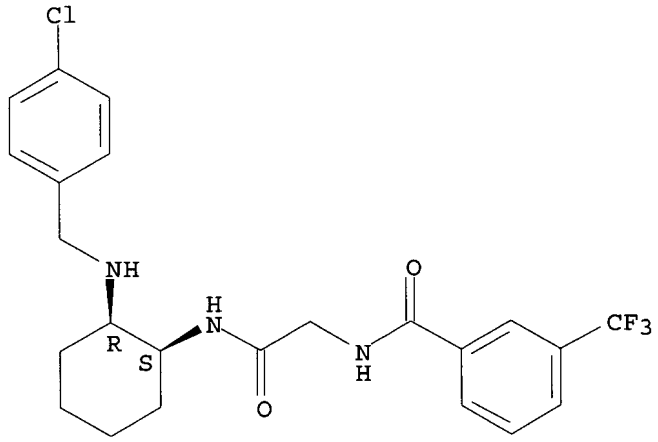
RN 445478-87-5 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[(2,4-dimethylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



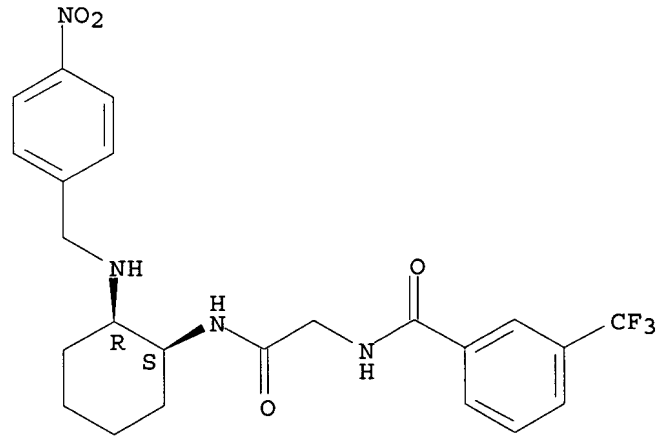
RN 445478-88-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[(4-chlorophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

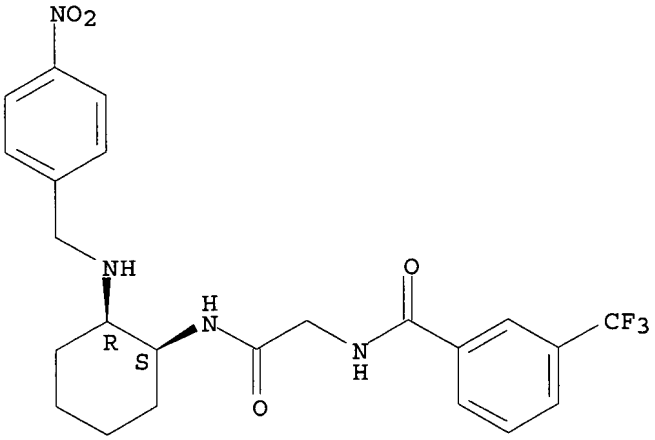
Relative stereochemistry.



RN 445478-89-7 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[(4-nitrophenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

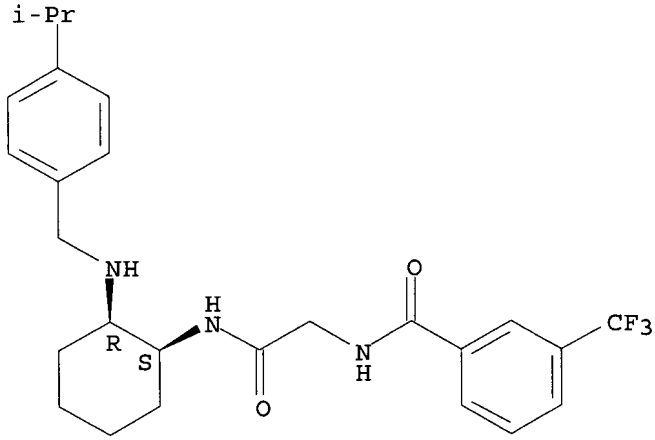
Relative stereochemistry.





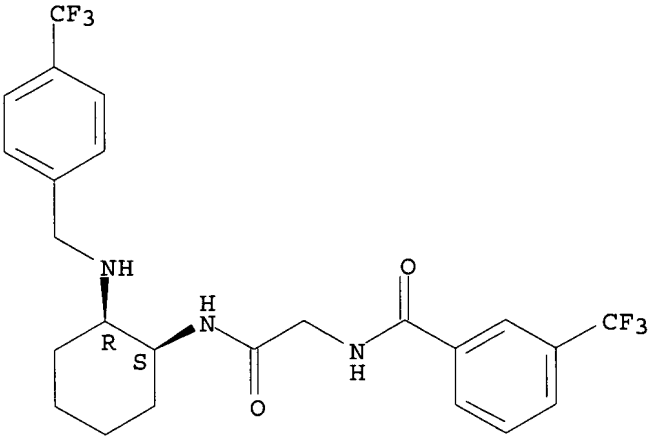
RN 445478-90-0 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[[4-(1-methylethyl)phenyl]methyl]amino]cycloh
exyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



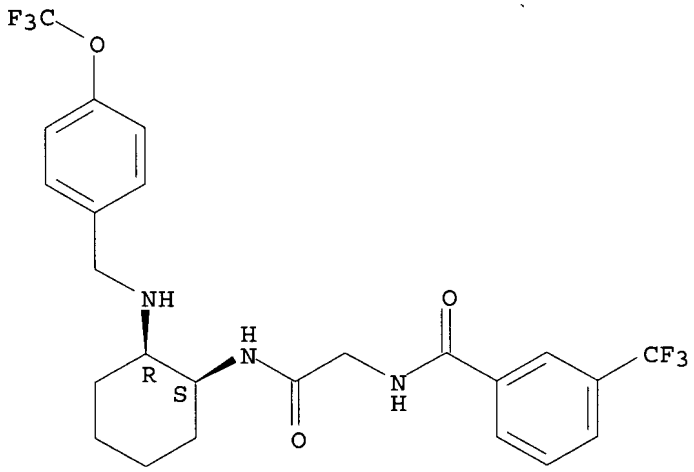
RN 445478-91-1 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[[4-(trifluoromethyl)phenyl]methyl]amin
o]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX
NAME)

Relative stereochemistry.



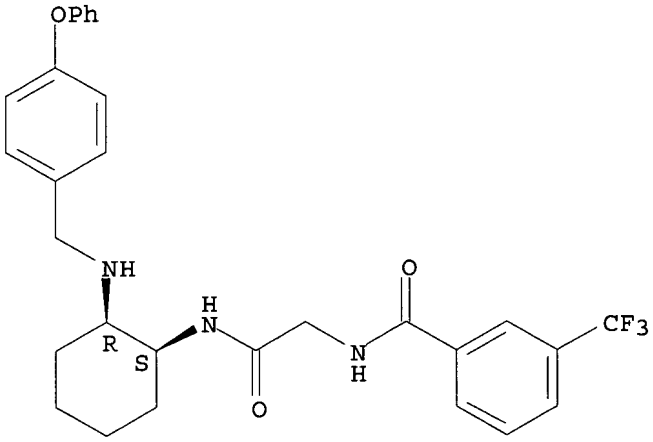
RN 445478-92-2 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[[4-(trifluoromethoxy)phenyl]methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



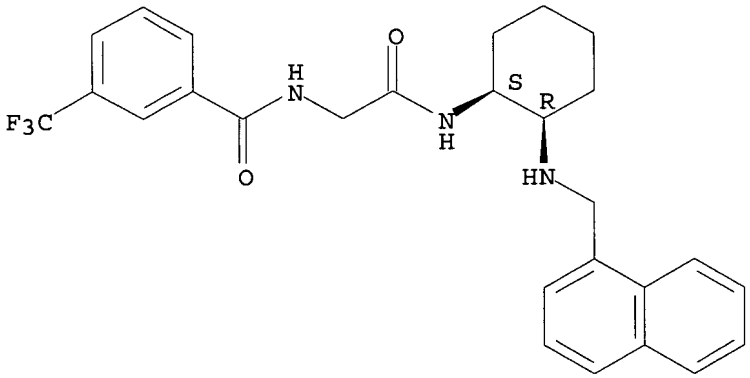
RN 445478-93-3 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[(4-phenoxyphenyl)methyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



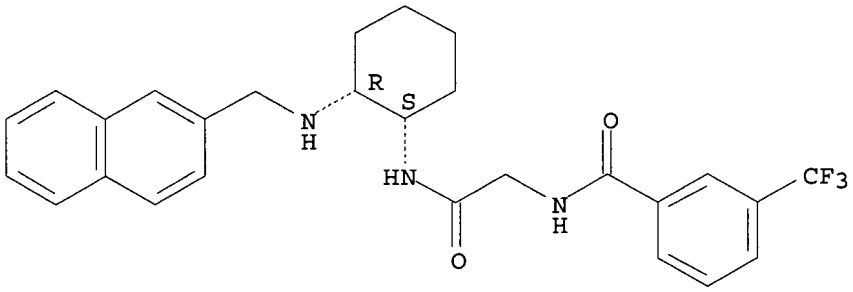
RN 445478-94-4 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(1-naphthalenylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



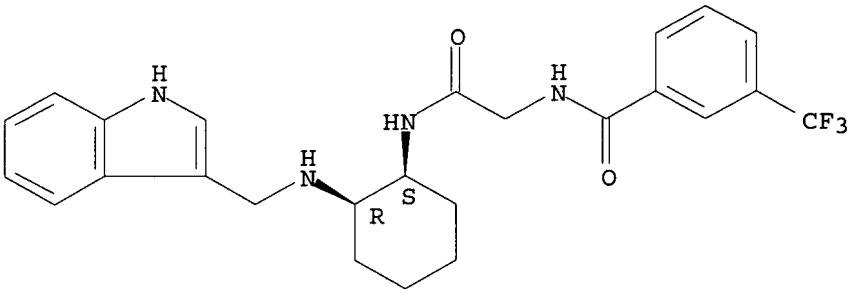
RN 445478-95-5 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(2-naphthalenylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



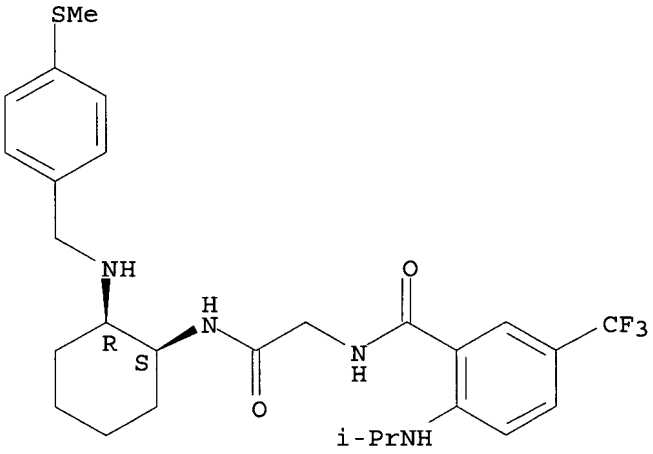
RN 445478-96-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(1H-indol-3-ylmethyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

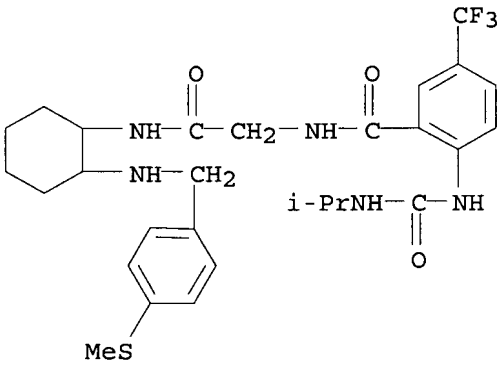


RN 445480-70-6 CAPLUS
CN Benzamide, 2-[(1-methylethyl)amino]-N-[2-[[(1R,2S)-2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

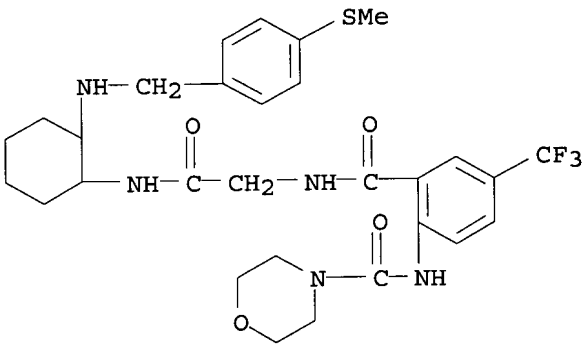
Relative stereochemistry.



RN 445480-72-8 CAPLUS
CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



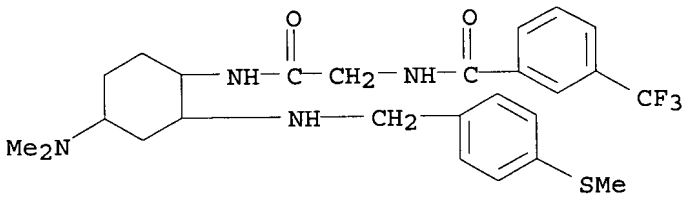
RN 445480-74-0 CAPLUS
CN 4-Morpholinecarboxamide, N-[2-[[[2-[[2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 445481-10-7 CAPLUS
CN Benzamide, N-[2-[[4-(dimethylamino)-2-[[[4-(methylthio)phenyl]methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

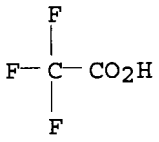
CM 1

CRN 445481-09-4
CMF C26 H33 F3 N4 O2 S



CM 2

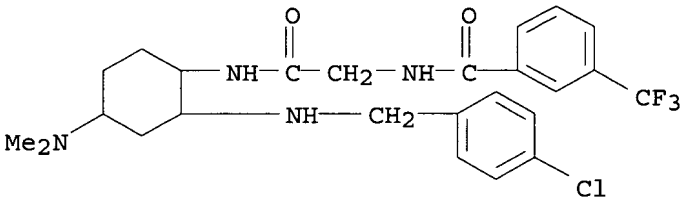
CRN 76-05-1
CMF C2 H F3 O2



RN 445481-16-3 CAPLUS
CN Benzamide, N-[2-[[2-[[(4-chlorophenyl)methyl]amino]-4-(dimethylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

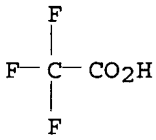
CM 1

CRN 445481-15-2
CMF C25 H30 Cl F3 N4 O2



CM 2

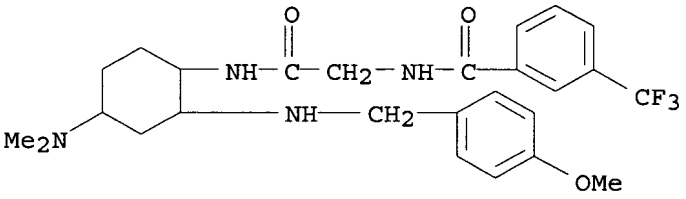
CRN 76-05-1
CMF C2 H F3 O2



RN 445481-18-5 CAPLUS
CN Benzamide, N-[2-[[4-(dimethylamino)-2-[[(4-methoxyphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

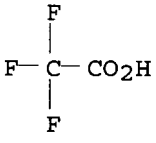
CM 1

CRN 445481-17-4
CMF C26 H33 F3 N4 O3



CM 2

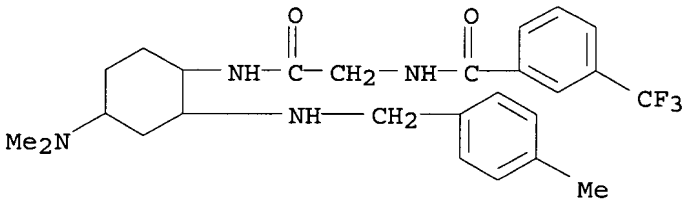
CRN 76-05-1
CMF C2 H F3 O2



RN 445481-20-9 CAPLUS
CN Benzamide, N-[2-[[4-(dimethylamino)-2-[[(4-methylphenyl)methyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

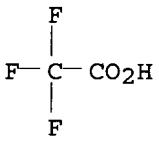
CM 1

CRN 445481-19-6
CMF C26 H33 F3 N4 O2

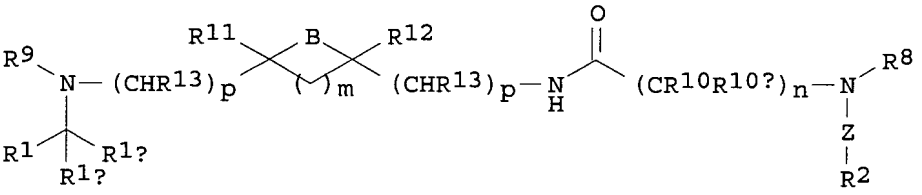


CM 2

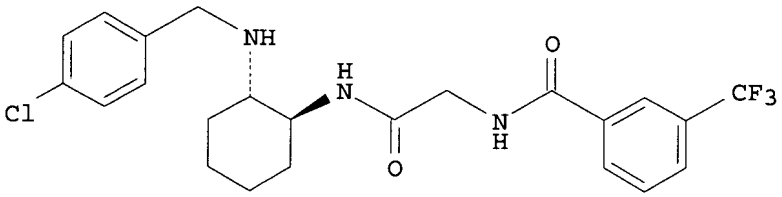
CRN 76-05-1
CMF C2 H F3 O2



GI



I



II

AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepd. as modulators of chemokine receptor activity, esp. monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addn. of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple sclerosis, atherosclerosis and asthma (no data).

L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:220576 CAPLUS
DOCUMENT NUMBER: 136:263160
TITLE: Preparation of azolylmethylaminotetrahydroquinolines and related compounds as chemokine receptor binding agents.
INVENTOR(S): Bridger, Gary; Skerlj, Renato; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di, Fluri Rosaria Maria
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 254 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022600	A2	20020321	WO 2001-CA1326	20010917
WO 2002022600	A3	20020510		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001091569	A5	20020326	AU 2001-91569	20010917
US 2003018046	A1	20030123	US 2001-957682	20010917

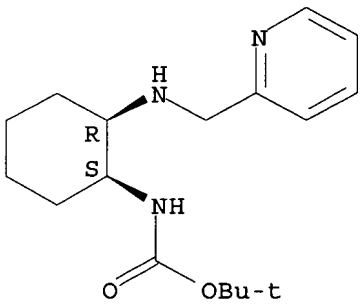
PRIORITY APPLN. INFO.:
US 2000-232891P P 20000915
US 2000-234510P P 20000922
WO 2001-CA1326 W 20010917

OTHER SOURCE(S): MARPAT 136:263160

IT **405059-09-8P 405175-27-1P 405175-37-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of azolylmethylaminotetrahydroquinolines and related compds. as chemokine receptor binding agents)

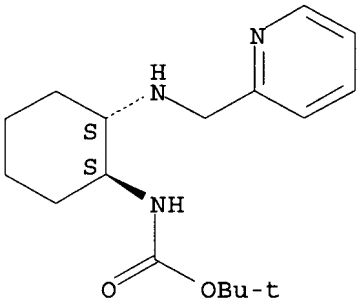
RN 405059-09-8 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[(2-pyridinylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



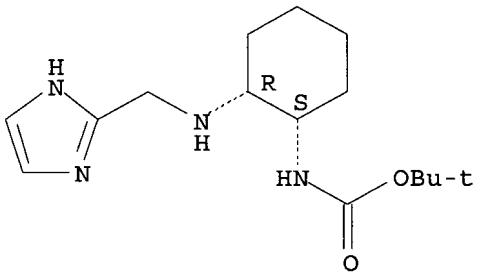
RN 405175-27-1 CAPLUS
CN Carbamic acid, [(1R,2R)-2-[(2-pyridinylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

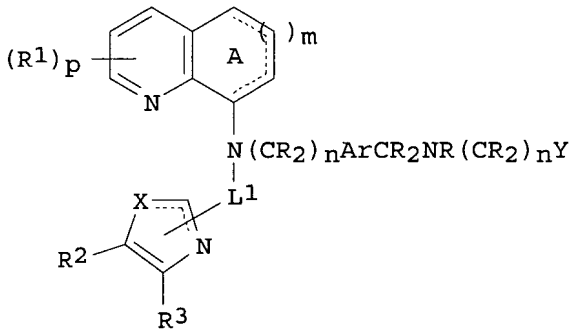


RN 405175-37-3 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[(1H-imidazol-2-ylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



I

AB Title compds. [I; ring A optionally contains N, O, S; dotted lines = optional unsatn.; R1, R2, R3 = non-interfering substituents; p = 0-4; m = 0-2; L1 = linker of 1.5-10 .ANG.; X = O, S, (substituted) C, N; Ar = aryl; n = 0-2; R = H, alkyl; Y = aryl, heteroaryl, heterocyclyl], were prepd. Thus, 5-trifluoromethyl-2-chloromethylbenzimidazole (prepn. given), N-(tert-butoxycarbonyl)-N-(2-pyridinylmethyl)-N'-(5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine, and diisopropylethylamine were stirred at 80.degree. in DMF for 16 h to yield N-(tert-butoxycarbonyl)-N-(2-pyridinylmethyl)-N'-(5-trifluoromethyl-1H-benzimidazol-2-ylmethyl)-N'-(5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine. Deprotection

with HBr in HOAc or dioxane gave N-(2-pyridinylmethyl)-N'-(5-trifluoromethyl-1H-benzimidazol-2-ylmethyl)-N'-(5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine hydrobromide. Several I inhibited HIV-1 replication in MT-4 cells with EC50<20 .mu.g/mL.

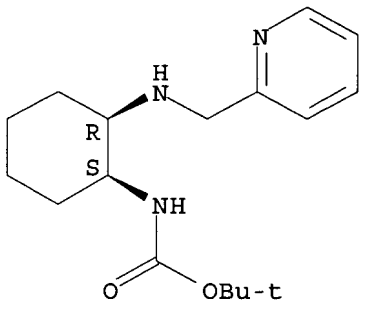
L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:220575 CAPLUS
DOCUMENT NUMBER: 136:263159
TITLE: Chemokine receptor-binding heterocyclic compounds, particularly (5,6,7,8-tetrahydroquinolin-8-yl)amino- and (1H-benzimidazol-2-yl)methyl-containing aromatic and heteroaromatic amides, useful for treating infection with HIV and FIV
INVENTOR(S): Bridger, Gary; Skerlj, Renato; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; McEachern, Ernest J.; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; Schols, Dominique; Smith, Christopher Dennis; Di Fluri, Rosaria Maria
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 146 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022599	A2	20020321	WO 2001-CA1325	20010917
WO 2002022599	A3	20020530		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001093551	A5	20020326	AU 2001-93551	20010917
US 2002147192	A1	20021010	US 2001-957654	20010917

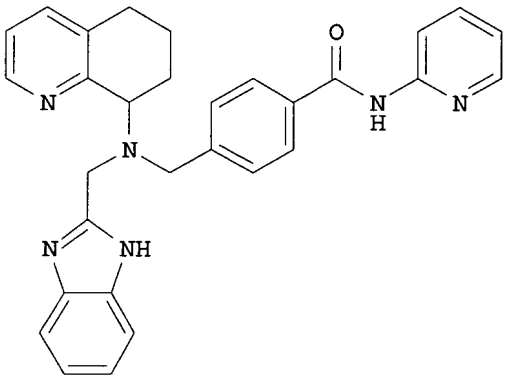
PRIORITY APPLN. INFO.: US 2000-233087P P 20000915
US 2000-234816P P 20000922
WO 2001-CA1325 W 20010917

OTHER SOURCE(S): MARPAT 136:263159
IT **405059-09-8P**, cis-N-(tert-Butoxycarbonyl)-N'-(2-pyridinylmethyl)cyclohexane-1,2-diamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of tetrahydroquinolinylamino- and benzimidazolylmethyl-contg. heterocyclic amides as chemokine receptor antagonists for treatment of HIV and FIV infection)
RN 405059-09-8 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[(2-pyridinylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



GI



II

AB Members of a class of (mostly tertiary) amines, contg. a multiplicity of heteroarom. substituents, and the salts and prodrug forms thereof, are useful as chemokine receptor modulators. In particular, compds. of formula X-L1-N(Z)-(CR12)n-Ar-L2-N(R2)-L3-Y (I) are disclosed [wherein: X = monocyclic (5-6 membered) or fused bicyclic (9-12 membered) (un)substituted ring system contg. at least 1 N, O, or S atom; Z = H, monocyclic (5-6 membered) or fused bicyclic (9-12 membered) (un)substituted ring system contg. at least 1 N, O, or S atom; Ar = (un)substituted arom. or heteroarom. ring; each of L1, L2, and L3 = bond, CO, SO2, or CH2, wherein at least 1 of L2 and L3 must comprise CO or SO2, and wherein L1 can also be alkylene (2-5C) wherein 1 or 2 C may optionally be replaced by N and which alkylene may itself optionally be substituted by a bridge alkylene (3-4C); L2 and L3 also may be, independently, SO2NH, CONH, SO2NHCH2 or CONHCH2; n = 0, 1, or 2; each R1 and R2 = H, straight or branched chain or cyclic alkyl (1-6C) which may optionally be substituted, and wherein R2 may be alkylene coupled to Y; and Y comprises at least 1 arom. or heteroarom. or other heterocyclic (un)substituted ring coupled directly to L3]. The compds. are useful for treatment of conditions which are modulated by the chemokine receptors CXCR4 and CCR5, and particularly for treatment of patients infected with HIV or FIV. Examples include 54 syntheses and 3 bioassays, and many addnl. compds. within the invention are listed. For instance, amidation of 4-(chloromethyl)benzoyl chloride with 2-aminopyridine (49%), followed by amination of the chloride with 8-[N-(2-nitrobenzenesulfonyl)amino]-5,6,7,8-tetrahydroquinoline (92%), removal of the 2-nitrobenzenesulfonyl group from the amine using PhSH and K2CO3 in DMF (93%), and finally N-alkylation of the amine with N-BOC-2-(chloromethyl)benzimidazole and deprotection (47%), gave title compd. II, designated AMD 9370. In a test for inhibition of Ca flux induced by the chemokine SDF-1.alpha. in SUP-T1 cells in vitro, 6 compds. including II gave > 20% inhibition at 20 .mu.g/mL. In a test for

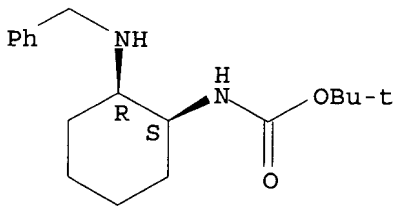
inhibition of NL4.3/IIIB (CXCR4-using) HIV-1 in MT-4 cells in vitro, 7 compds. including II exhibited EC50 values < 20 .mu.g/mL. The compds. also inhibited BaL (CCR5-using) HIV-1 similarly.

L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:747751 CAPLUS
DOCUMENT NUMBER: 135:303902
TITLE: Preparation of ethylenediamine and 1,2-cycloalkanediamine derivatives as inhibitors of activated blood coagulation factor X
INVENTOR(S): Yoshino, Toshiharu; Nagata, Tsutomu; Haginoya, Noriyasu; Yoshikawa, Kenji; Kanno, Hideyuki; Nagamochi, Masatoshi
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 481 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001074774	A1	20011011	WO 2001-JP2945	20010405
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001046835	A5	20011015	AU 2001-46835	20010405
EP 1270557	A1	20030102	EP 2001-919784	20010405
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2002004766	A	20021128	NO 2002-4766	20021003

PRIORITY APPLN. INFO.: JP 2000-108047 A 20000405
WO 2001-JP2945 W 20010405
OTHER SOURCE(S): MARPAT 135:303902
IT **365996-39-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of ethylenediamine and cycloalkanediamine derivs. as inhibitors of activated blood coagulation factor X for treatment of thrombosis and embolism)
RN 365996-39-0 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[(phenylmethyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB Compds. of the general formula (1): Q1-Q2-CO-N(R1)-Q3-N(R2)-T1-Q4 [R1, R2 = H, OH, alkyl, alkoxy; Q1 = (un)substituted and (un)satd. 5- to

6-membered cyclohydrocarbyl or heterocyclyl or bi- or tricyclic condensed heterocyclyl; Q2 = bond, linear or branched alkyl C1-6 alkylene, C2-6 alkenylene, or C2-6 alkynylene, N-alkyl-(un)substituted NH or NH(CH2)m, (un)substituted and (un)satd. divalent 5- to 6-membered cyclic hydrocarbon or heterocycle or bi- or tricyclic condensed heterocycle group; Q3 = CR5R6CR7R8 (wherein R5, R6, R7, R8 = H, HO, halo, haloalkyl, cyano, cyanoalkyl, acyl, acylalkyl, alkyl, alkenyl, alkynyl, alkoxy, alkoxyalkyl, hydroxyalkyl, CO2H, carboxyalkyl, etc.), Q (wherein Q5 = C1-8 alkylene or C2-8 alkenylene; R9 and R10 are substituted on the carbon atoms of the ring contg. Q5 and represent H, OH, alkyl, alkenyl, alkynyl, halo, haloalkyl, cyano, cyanoalkyl, NH2, aminoalkyl, N-alkylaminoalkyl, etc.); Q4 = (un)substituted aryl, arylalkenyl, heteroaryl, or heteroarylalkenyl, (un)substituted and (un)satd. bi- or tricyclic condensed hydrocarbyl or condensed heterocyclyl; T1 = CO, SO2] are prepd. Also claimed are drugs which contain these compds. and are efficacious for thrombosis and embolism. Thus, (.+-.)-cis-N1 (or N2)-[(5-chloroindol-2-yl)carbonyl]-4,4-(1,2-ethylenedioxy)-1,2-cycloalkanediamine was condensed with 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine-2-carboxylic acid using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and 1-hydroxybenzotriazole monohydrate in DMF at room temp. overnight to give (.+-.)-cis-N1 (or N2)-[(5-chloroindol-2-yl)carbonyl]-4,4-(1,2-ethylenedioxy)-N2 (or N1)-[(5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]-1,2-cyclohexanediamine (II). II in vitro showed IC50 of 1.4 nM .mu.g/mL against human FXa.

REFERENCE COUNT: 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:713294 CAPLUS

DOCUMENT NUMBER: 135:257169

TITLE: Preparation of cyclic .beta.-amino acid derivatives as inhibitors of matrix metalloproteases and TNF-.alpha.

INVENTOR(S): Duan, Jingwu; Ott, Gregory; Chen, Linhua; Lu, Zhonghui; Maduskuie, Thomas P., Jr.; Voss, Matthew E.; Xue, Chu-Biao

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 298 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001070673	A2	20010927	WO 2001-US8334	20010315
WO 2001070673	A3	20020314		
W: AT, AU, BR, CA, CH, CN, CZ, DE, DK, EE, ES, FI, HU, IN, JP, KR, LT, LU, LV, MX, NZ, PL, PT, RO, SE, SG, SI, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1263755	A2	20021211	EP 2001-924170	20010315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR				
US 2002016336	A1	20020207	US 2001-811233	20010316

PRIORITY APPLN. INFO.:
US 2000-190182P P 20000317
US 2000-233373P P 20000918
US 2000-255539P P 20001214
WO 2001-US8334 W 20010315

OTHER SOURCE(S): MARPAT 135:257169

IT **362491-59-6P**

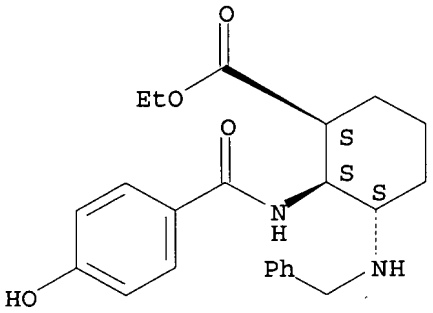
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(prepn. of cyclic .beta.-amino acid derivs. as inhibitors of matrix metalloproteases and TNF-.alpha.)

RN 362491-59-6 CAPLUS

CN Cyclohexanecarboxylic acid, 2-[(4-hydroxybenzoyl)amino]-3-[(phenylmethyl)amino]-, ethyl ester, (1R,2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB Novel cyclic .beta.-amino acid derivs. A-CRR2aCRR2bNR1CO-Z-Ua-Xa-Ya-Za [A = CO2H, CH2CO2H, SH, CH2SH, S(O)Ra:NH (Ra = H, alkyl, Ph, benzyl), P(O)(OH)2, etc.; CRCR is a substituted 3-13 membered nonarom. carbocyclic or heterocyclic ring; Z is absent or substituted C3-13 carbocycle or 5-14 membered heterocycle; Ua is absent or O, NRa1 (Ra1 = H, alkyl), CO, CO2, O2C, CONRa1, S(O)p (p = 0-2), etc.; Xa is absent or C1-10 alkylene, C2-10 alkenylene or alkynylene; Ya is absent or O, NRa1, S(O)p or CO; Za is H, substituted C3-13 carbocycle or 5-14 membered heterocycle; R1 is H, C1-4 alkyl, Ph, benzyl; R2a is H, C1-6 alkyl, ORa, NRaRa1 or S(O)pRa; R2b is H, C1-6 alkyl (with provisos)] or pharmaceutically acceptable salts were prepd. as metalloprotease and TNF-.alpha. inhibitors. Thus, (3S,4S)-N-hydroxy-1-isopropyl-4-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-3-pyrrolidinecarboxamide was prepd. by a multistep procedure starting with condensation of benzyl Me maleate, glycine, and paraformaldehyde to form 3,4-pyrroledicarboxylate diester and involving amidation of 4-[(2-methyl-4-quinolinyl)methoxy]benzoic acid.

L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:836249 CAPLUS

DOCUMENT NUMBER: 134:147352

TITLE: Amide catalysts with tetradentate ligands and the asymmetric transfer hydrogenation of carbonyl compounds

AUTHOR(S): Marson, C. M.; Schwarz, I.

CORPORATE SOURCE: Department of Chemistry, University College London, Christopher Ingold Laboratories, London, WC1H OAJ, UK

SOURCE: Tetrahedron Letters (2000), 41(46), 8999-9003
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

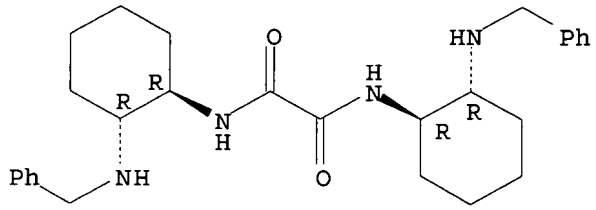
OTHER SOURCE(S): CASREACT 134:147352

IT **323187-53-7P 323187-54-8P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of amidic tetradentate ligands as catalysts for asym. transfer hydrogenation of carbonyl compds.)

RN 323187-53-7 CAPLUS

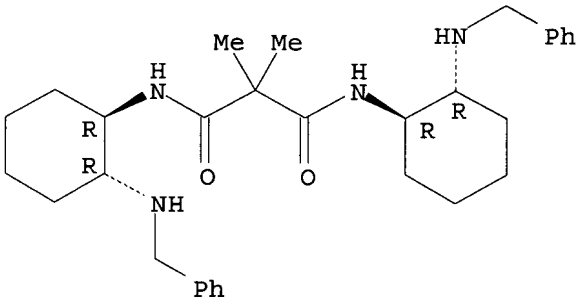
CN Ethanediamide, N,N'-bis[(1R,2R)-2-[(phenylmethyl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 323187-54-8 CAPLUS
CN Propanediamide, 2,2-dimethyl-N,N'-bis[(1R,2R)-2-[(phenylmethyl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

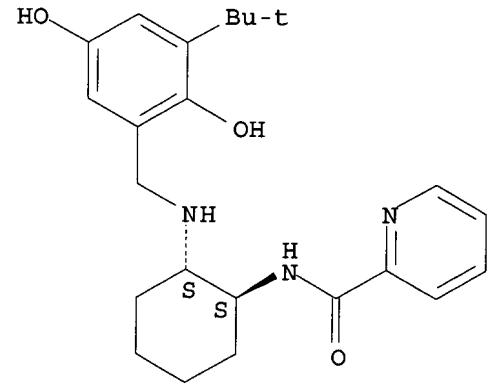
Absolute stereochemistry.



AB Amidic tetradentate catalysts comprising two trans-1,2-cyclohexanediamine units linked via a dicarbonyl spacer are shown to provide useful enantiomeric excesses in the asym. transfer hydrogenation from propan-2-ol to arom. ketones. N-benzylation of the terminal amino groups results, in several cases, in reversal of the abs. configuration of the major product.
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

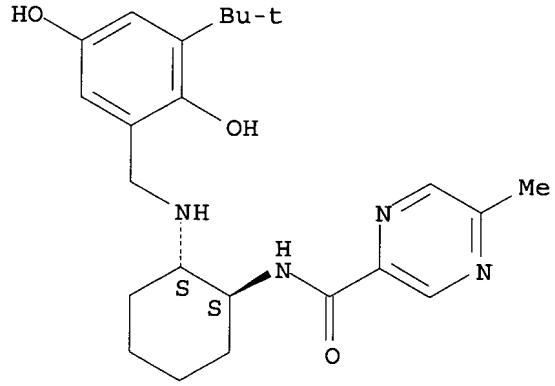
L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:251901 CAPLUS
DOCUMENT NUMBER: 131:10019
TITLE: Discovery of novel catalysts for alkene epoxidation from metal-binding combinatorial libraries
AUTHOR(S): Francis, Matthew B.; Jacobsen, Eric N.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology and Institute of Chemistry and Cellular Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Angewandte Chemie, International Edition (1999), 38(7), 937-941
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **225666-16-0P 225666-17-1P 225666-18-2P 225666-19-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(imine ligands prepd. on solid phase for the discovery of active catalysts in the epoxidn. of trans-.beta.-methylstyrene, cleaved from solid phase and characterized)
RN 225666-16-0 CAPLUS
CN 2-Pyridinecarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



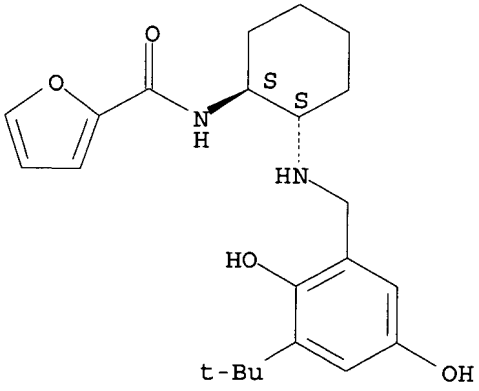
RN 225666-17-1 CAPLUS
CN Pyrazinecarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



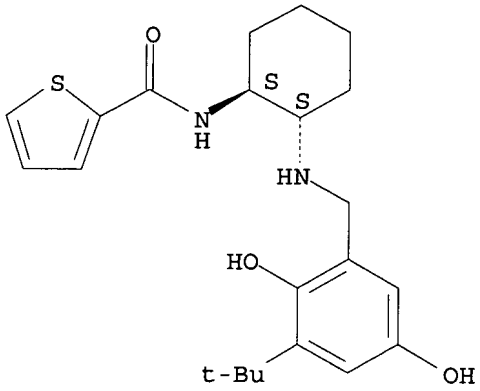
RN 225666-18-2 CAPLUS
CN 2-Furancarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

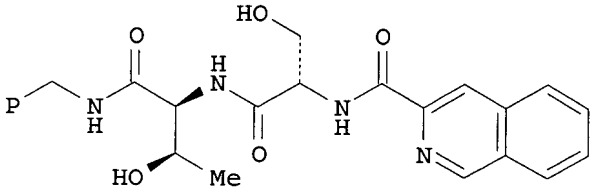


RN 225666-19-3 CAPLUS
CN 2-Thiophenecarboxamide, N-[(1S,2S)-2-[[[3-(1,1-dimethylethyl)-2,5-dihydroxyphenyl]methyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



I

AB A combinatorial library of imine ligands is prepd. on solid support and tested for activity in the stereoselective epoxidn. of trans-.beta.-methylstyrene in the presence of metal salts and hydrogen peroxide. The library consisted in part of amino acids (asparagine, cysteine, histidine, methionine, or serine) linked at their N-termini to cis-aminoindenol, trans-diaminocyclohexane, or serine whose free amino groups were used to form imines or amides with aldehydes or carboxylic acids. A library of salen ligands with different imine groups was also prepd. FeCl2 was the most effective metal precursor with the libraries in epoxidns. with H2O2. Serine or cysteine worked best as the C-terminal amino acids for epoxidn. ligands, while 2-pyridinecarboxaldehyde and 2-pyridinecarboxylic acid were the most effective capping reagents for the ligands. Polymer-bound ligand I (P = polymer) was treated with a 0.02M soln. of FeCl2 in 4:1 THF:MeOH and agitated and purified until the THF:MeOH rinses were clear; treatment of trans-.beta.-methylstyrene in 1:1 CH2Cl2:Me3COH with the resin-bound FeCl2 complex of I followed by addn. of 1.5 equiv. of 30% H2O2 gave (R,R)-trans-.beta.-methylstyrene oxide with 78% conversion, 69% yield, and in 20% ee.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:103032 CAPLUS
DOCUMENT NUMBER: 94:103032
TITLE: Analgesic N-(2-(furylmethylamino and 2-thienylmethylamino)cycloaliphatic)benzamides
INVENTOR(S): Szmuszkovic, Jacob
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: U.S., 33 pp. Cont.-in-part of U.S. 4,153,717.
CODEN: USXXAM

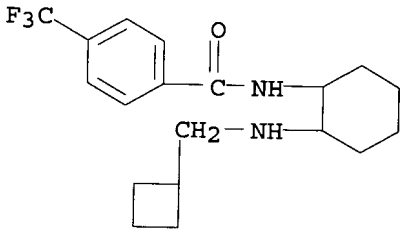
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4215114	A	19800729	US 1979-17679	19790305
US 4098904	A	19780704	US 1976-741467	19761112
CA 1072558	A1	19800226	CA 1977-287430	19770926
US 4153717	A	19790508	US 1978-906271	19780515
US 4192885	A	19800311	US 1979-18550	19790308

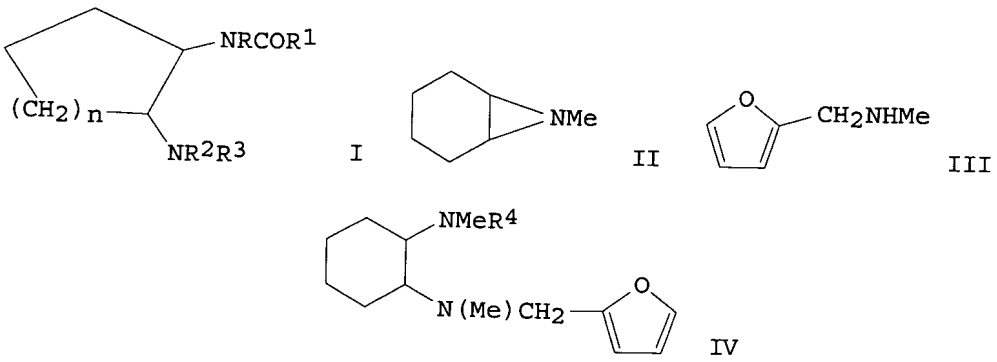
PRIORITY APPLN. INFO.:

US	1976-741467	19761112
US	1978-906271	19780515
US	1978-904477	19780510
CA	1979-287430	19790906

IT **75570-55-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 75570-55-7 CAPLUS
CN Benzamide, N-[2-[(cyclobutylmethyl)amino]cyclohexyl]-4-(trifluoromethyl)-(9CI) (CA INDEX NAME)



GI



AB Analgesic (no data) cycloaliph. benzamides I (n = 1-8; R = H, alkyl; R1 = optionally substituted Ph; R2 = alkyl; R3 = furfuryl, thenyl) were prepd. Thus, heating II with furfurylamine III gave IV (R4 = H) which was acylated using 3,4-Cl2C6H3COCl to IV (R4 = COC6H3Cl2-3,4).

=> log y
COST IN U.S. DOLLARS

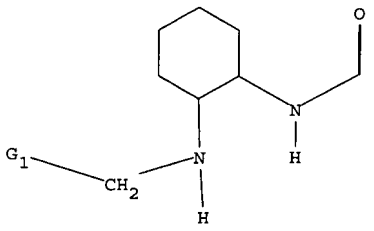
	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	37.12	186.28

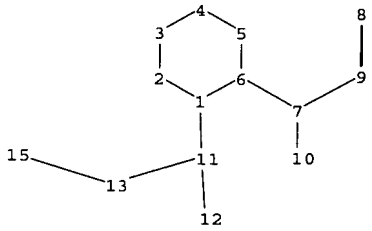
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	-5.21	-5.21

STN INTERNATIONAL LOGOFF AT 10:57:53 ON 13 MAR 2003

\STNEXP4\QUERIES\10027644.str





ain nodes :
7 8 9 10 11 12 13 15
ng nodes :
1 2 3 4 5 6
ain bonds :
1-11 6-7 7-9 7-10 8-9 11-12 11-13 13-15
ng bonds :
1-2 1-6 2-3 3-4 4-5 5-6
act/norm bonds :
1-11 6-7 7-9 8-9 13-15
act bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-10 11-12 11-13
olated ring systems :
containing 1 :

:Cb,Hy

tch level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 15:CLASS